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13. ABSTRACT (Maximum 200 words)

This project combines analytic and computational investigations to understand the dynamics of elastic-plastic deformation of granular materials, particularly issues related to the formation of shearbands. Roughly speaking, shearbands form when the governing equations cease to be well-posed. Our research examines the issue of well-posedness, loss of hyperbolicity, and regularization. This final report summarizes our work on (*i*) computation of deformation and formation of shear bands in granular material; (*ii*) analysis of a gradient theory of granular plasticity; (*iii*) related elastic and visco-elastic systems of PDE which may lose hyperbolicity.

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Computational Deformation and Shearbands We begin by summarizing our work on shearband formation [5]; the second sub-section outlines our work on adaptative implicit-explicit methods for elastic-plastic deformation [7].

Shearbands The equations governing the motion of a granular continuum are the balance laws for mass and momentum. A particularly simple model to study is the anti-plane shearing of a continuum. If $(x,\ y)$ denote the in-plane coordinates, z the direction orthogonal to this plane, and v the velocity in the z-direction, then the continuity equation is identically satisfied with a constant density, and the only non-trivial momentum equation is for the z-direction,

$$\partial_t v \ + \ {c_e}^2 \partial_x T_{xz} \ + \ {c_e}^2 \partial_y T_{yz} \ = \ 0. \qquad (1.1a)$$

T is the Cauchy stress tensor, where compressive stresses are taken to be positive.

We now must augment (1.1a) with suitable constitutive information detailing the evolution of the stresses T_{xz} and T_{yz}. To this end, we follow Schaeffer [10] and adopt a von-Mises type Yield condition with strain-hardening, and a possibly non-associative flow rule.

$$\partial_t \sigma \ + \ [I - H(\sigma, \bar{\sigma}) \Re \sigma] \ \nabla v \ = \ 0. \qquad (1.1b)$$

Here, $\sigma = (T_{xz},\ T_{yz})^*$ and the $*$ denotes transpose. The rotation $\Re\sigma$ gives the direction of the strain-rate tensor, where

$$\Re \ = \ \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix}$$

and α is the angle of non-associativity. Finally, $H(\sigma, \bar{\sigma})$ contains the constitutive information related to loading and hardening:

$$H \ = <\ell> \frac{\sigma^*}{h(\bar{\sigma}) + |\bar{\sigma}|^2 \cos(\alpha)}$$

where $\bar{\sigma}(x) = max_{0 \le s \le t}\ |\sigma(x,s)|$ is the maximum previous stress level (and is an equivalent measure as the total accumulated shear strain γ). A typical model for the hardening function is $h(\bar{\sigma}) = h_0\sqrt{1 - |\bar{\sigma}|}$. The elastic components are modeled by linear elasticity. The switch $<\ell>$ is 1 if the material is loading plastically (i.e. if $|\sigma(x,t)| = |\bar{\sigma}(x)|$), and 0 otherwise.

In writing the equations above, we have non-dimensionalized relative to parameters typical in a biaxial laboratory test. In this setting, the maximum possible total stress $|\sigma|_{max} = 1$ and the elastic wave speed $c_e \approx 10^6$. In order to make the calculations feasible with a reasonable expenditure of computing resources, we compute with an artificial wavespeed of 1.

It is convenient to examine the one-dimensional system to get a feeling for the fundamental dynamics of the system. If we assume $\partial_y = 0$, the resulting system is hyperbolic whenever $|\bar{\sigma}| < \bar{\sigma}_{crit}$, where the critical stress $\bar{\sigma}_{crit}$ depends on the degree of non-associativity. In particular, $\bar{\sigma}_{crit} = 1$ when $\alpha = 0$ (i.e., the system is always hyperbolic when the flow rule is associative) and $\bar{\sigma}_{crit} < 1$ when $\alpha \neq 0$. Similar statements hold in the two dimensional setting.

Roughly speaking, a shearband forms whenever any one component of stress reaches a maximum and begins to decrease, even if the total stress (e.g. the squared norm of the stress tensor) is still increasing.

Before equations (1.1) lose hyperbolicity, the system consists of a single conservation law for momentum balance, and two stress-rate equations which are not in conservation form. The paper [5] details a Godunov-type scheme which integrates the governing equations numerically, allowing for loss of hyperbolicity and the formation of shearbands. The Godunov scheme is related to ideas in [1, 11]

Our basic scheme consists of four parts: (*i*) monotone slope determination; (*ii*) characteristic tracing; (*iii*) wave interaction (*iv*) conservative update of momentum and time-centered stress update. This basic scheme must be amended wherever hyperbolicity is lost. In that case, a shearband is assumed to form in a cell which experiences change-of-type. This shearband is treated as an internal boundary; plausible boundary conditions proposed by Schaeffer [10] are imposed at the boundary and characteristic tracing is used to update the dependent variables on each side of this boundary. Integration in the rest of the domain is not affected.

Results of our computations illustrate how the loss of hyperbolicity at one location promotes unloading nearby, thus localizing deformation into a shearband. This unloading provides a nonlinear 'regularization', in that loss of hyperbolicity does not lead to global blow-up of the solution. Rather, a smooth solution may lose differentiability once the system loses hyperbolicity, but the strains remain piecewise smooth with jump discontinuities. Further computational experiments are in progress, allowing for closer examination of the phenomenon of unloading.

Implicit-Explicit Computations As mentioned above, the speed of elastic waves in a granular material are on the order of 10^6 cm./sec. In computations, this large wavespeed imposes a stringent constraint on the allowable timestep for an explicit calculation, a timestep too small for a fully explicit numerical simulation of an experimental biaxial test. To overcome this stability constraint, we are developing an Adaptatively Implicit-Explicit (AIE) Godunov method for wave propagation [7]. The motivating feature is this work is that most elastic waves are weak and do not contribute substantially to the dynamics. The most important waves are (1) waves of strong plastic response, and (2) unloading waves from the shearband.

Previously, Fryxell et. al. [4] developed an implicit Godunov method for gas dynamics; this method is fully second-order in time, using a trapezoidal rule integration in time. The price paid for second-order accuracy is that the linear algebra system to be solved at each gridpoint consists of 2N equations, where N is the number of conservation equations to be solved. Further, the desire for monotonicity limits the timestep to approximately twice the explicit timestep. This timestep limit is still too small for our elastic-plastic problem, and the role of plasticity in our system requires new ideas.

Following ideas of P. Colella and J. Trangenstein, we have begun a program to develop the AIE method for elastic-plastic deformation. The idea is to switch smoothly between explicit and implicit time-integration for each wave, independent of other waves. For waves which are computed explicitly, the method proceeds as above; for waves which are computed implicitly, we reduce to first-order accuracy in time (currently using backwards Euler) and space (no characteristic tracing). We use the Godunov methodology of averaging (in space) the solution of Riemann problems to ensure good dispersion characteristics. While the backward Euler time integration may dampen some waves which should not decay, this integrator does give a monotone (in time) solution. Further, the linear algebra problem consists of N equations at each gridpoint.

To date, we have written an AIE code for solving the elastic-plastic model of Antman [1]. This model consists of 2 conservation laws (in 1 space dimension), plus a single ODE for the accumulated shear. The fundamental simplification of this model is that the system is always strictly hyperbolic. We have made comparisons with Trangenstein's analytic solution to the Riemann problem for this model, and with his explicit Godunov calculations. While our current version works well for relatively weak-wave solutions and small multiples of the explicit timestep (order 5), performance for strong-wave solutions and very large timesteps is less satisfactory. We are currently working on an iteration scheme to overcome these limitations. (Note: Trangenstein's explicit computations also degraded for strong-wave solutions, and he modified the wave tracing part of the algorithm to obtain better performance. We are examining how his modifications may be adapted into our method.)

Our primary goal in developing AIE is to to solve the anti-plane shear model. We are studying the modifications necessary to adapt our current code for this problem. The most vexing difficulty is how to accurately (i.e. explicitly) capture unloading waves near the shearband while treating other elastic waves implicitly. Our current strategy is to use AIE for the initial loading of the sample, until the maximum stress is large (say $|\bar{\sigma}| \approx 0.75\bar{\sigma}_{crit}$), and then switch to fully a explicit integration, to capture shearbands and unloading waves accurately.

Gradient Theory Significant work is required to understand the true nature of the shear band before physically "correct" jump conditions can be applied. Schaeffer's suggestion in [10] is to apply the same constitutive relations to the rapidly shearing material inside the band but include a new (phenomenological) lengthscale i.e. the band thickness. An alternative approach is to identify the the most important dissipative processes, which provide a high frequency cutoff to the strain-rate blow-up. Then it may be possible to derive jump conditions in the limit as the strength of these dissipative processes approaches zero.

We have studied continuum theories which provide a dissipation mechanism, with the intention of (*i*) examining well-posedness of these models, and (*ii*) deriving jump conditions. To this end, we began with a Cosserat model as a possible regularization method. The couple-stresses in the Cosserat continuum do provide a high-frequency cutoff and regularization for shearing motions. But the model fails to provide regularization for dilation.

Therefore we have examined higher-order gradient theories as a potential model (see [12]). This theory consists of mass and momentum balance, plus constitutive equations which can be written as

$$|devT| = \mu(\gamma, \Delta\gamma) \tag{2a}$$

$$devV^{(p)} = \lambda\frac{devT}{|devT|} \tag{2b}$$

$$trV^{(p)} = \beta(\gamma, \Delta\gamma) \ . \tag{2c}$$

These equations express the yield condition, flow rule, and dilatancy, depending on the accumulated shear, γ, and the Laplacian $\Delta\gamma$. The accumulated shear evolves according to $\partial_t\gamma = |devV^{(p)}|$. V is the strain rate,

$$V_{ij} = -\frac{1}{2}(\partial_i v_j + \partial_j v_i)$$

and $V^{(p)}$ denotes the plastic part of the strain-rate. Also, trV denotes the trace of V, $trV = V_{ii}$, and the deviator $devV = V - (trV)I$ where I is the identity matrix. The resulting system of equations differs from a more conventional Flow Theory of plasticity in that a PDE for γ must be solved.

The analysis of simple shear is completed, and analysis of general flow is partially completed [8]. In the case of simple shear with a velocity u depending on the single space variable y, the governing equations may be written

$$\partial_t u - \frac{1}{\sqrt{2}}\partial_y \mu(\gamma, \partial_{yy}\gamma) = 0$$

$$\partial_t \gamma - \frac{1}{\sqrt{2}}\partial_y u = 0$$

Linearizing, looking for exponential solutions $e^{iy\xi+\lambda(\xi)t}$ and solving the resulting eigenvalue problem, we find $\lambda = \pm\frac{|\xi|}{\sqrt{2}}\sqrt{\xi^2\mu_2 - \mu_1}$, where μ_1 and μ_2 are the partial derivitives of μ with respect to its first and second arguments. In classical Flow Theory of plasticity, μ_1 is positive until a critical value of the accumulated shear is reached and then becomes negative; this non-monotonicity is the source of ill-posedness and shearband formation. If $\mu_2 < 0$, the incorporation of the higher order gradient regularizes the equations and leads to a well-posed system. However the system may be unstable for a range of wavenumbers ξ, and concentrate deformation in a narrow region.

Further analysis of the simple shear problem also shows that the system exhibits shearband-like solutions, similar to those found in [2].

After completing the calculation showing well-posedness, we plan to examine whether this theory can be used in an anti-plane shearing problem, as a means of deriving jump conditions.

Related Systems We have studied two issues related to the well-posedness of elastic-plastic deformation problems. The first issue concerns constitutive relations with rotational symmetry; the second, a relaxation phenomenon.

Rotational Symmetry The issue of isotropy within hyperelastic-plastic models in multiple dimensions is important. In particular, if the stresses are assumed to be rotationally invariant, then the governing equations are not strictly hyperbolic. The origin in state space is an umbilic point. Existence of an umbilic point becomes a serious issue when motions which include the origin are permitted. In particular, the usual high order techniques for solving hyperbolic conservation laws fail for such motions. With H. Freistuhler we are examining this issue [3].

For rotationally invariant materials, the stress is usually taken to be a function of the strain of the form

$$T(U) = \phi(|U|^2)U.$$

We examined a model of this kind, numerically solving the Riemann problem for the 2×2 system

$$\partial_t U + \partial_x(|U|^2 U) = 0 \tag{3}$$

where $U = (u, v)$. (Remark: There is a precise isomorphism between the wave patterns of (3) and (a specific) part of the wave pattern of any generic rotationally degenerate system of hyperbolic conservation laws, including isotropic, neo-Hookian elasticity.) It is unclear what additional effects plastic yielding will have on the computational solution.

Equation (3) is hyperbolic, with eigenvalues $\lambda_a = |U|^2$ and $\lambda_r = 3|U|^2$, and right eigenvectors $r_a = (-v, u)$ and $r_r = (u, v)$. Note: the slow azimuthal field is linearly degenerate in the sense of Lax, while the fast radial field is nonlinear away from the origin.

We solved the Riemann problem for (3) using two different types of numerical method, viz. a random choice scheme, and a Godunov scheme. The random choice method is only first order accurate in space and time, but introduces no artificial dissipation into the calculation. In contrast, the Godunov scheme we implemented is second order accurate, but incorporates a selective amount of diffusion into the different wave families. This diffusion corrupts the solution for special Riemann data. Let us explain this last statement.

For Riemann data U_l and U_r which is colinear and lie on opposite sides of the origin, there are two possible constructions of a solution. For a specific example, let us consider

$$U_l = (u_l, v_l) = (1,0) \qquad U_r = (u_r, v_r) = (-1,0)$$

One may construct a solution which follows the azimuthal field around from (1,0) to (-1,0), establishing a contact discontinuity. Also, one could consider the reduced system

$$\partial_t u + \partial_x u^3 \qquad v = 0$$

The solution of this reduced system follows the construction of Wendroff and Liu, and u undergoes a composite shock-rarefaction.

These different constructs point to a non-uniqueness in the solution operator for (3). In particular, we have demonstrated in [3] that, for nearly colinear Riemann data, the Godunov scheme approximately mimics the reduced-system construction, while the random choice scheme (by design) mimics the centered wave construction.

We believe this result illustrated the difficulties to be overcome in the numerical simulation of hyperelastic material models. This project is continuing, as Freistuhler and I study other numerical algorithms for rotationally invariant systems, in particular, questions of convergence for the Cauchy problem.

Viscoelastic Relaxation Work is in progress studying relaxation mechanisms. Consider the system

$$\partial_t u - \partial_x v = 0 \tag{4a}$$

$$\partial_t v - \partial_x P = 0 \ . \tag{4b}$$

If we provide constitutive information $P = P(u, v)$, the system is closed and is used as a model of deformation of an elastic bar. With $P = P_{ref} = u^3/3-u$, the system is hyperbolic whenever $|u| > 1$ and elliptic otherwise. This model is used to study change-of-phase in elastic materials. To prove existence of solutions, Eq. 4a-4b must be augmented with an admissibility criterion describing the types of discontinuities allowed in the solution. A result of

Shearer shows non-uniqueness of the solution for certain initial data. That is, different solutions emerge for initial data in a special region in the (u, v)-plane. One solution consists of two rarefaction waves coupled with two phase jumps, and is obtained in the limit when a viscosity or viscosity-capillarity regularization is used.

We are examining a different kind of regularization. Assume P is described by its own evolution equation, given by a viscoelastic relaxation constitutive model, and augment Eq. 4a and 4b with

$$\partial_t P + E^2 \partial_t u = \frac{-(P - P_{ref})}{\tau} \tag{4c}$$

where τ is a relaxation time. In what sense do solutions of the relaxation system Eq. 4a-c converge, as $\tau \to 0$, to solutions of the p-system Eq. 4a-4b, with $P = P_{ref}$? As part of his Ph D. thesis, Mr. Yigong Ni is studying this problem numerically [9], and he has partial analytic results on convergence as $\tau \to 0$. One particular numerical finding is that the relaxation limit solution is not the same as the viscous regularization solution. The analysis gives a partial answer to the question of convergence for smooth solutions, and also provides asymptotic behavior near discontinuities. These result will be important in our granular flow work, when considering viscoplastic constitutive relations (i.e. relaxation systems such as Eq. 4, with plasticity included).

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